

code: https://github.com/anandpratap/flame_1d

I. INTRODUCTION

The governing equations are,

$$\dot{m} \frac{\partial T}{\partial x} = \frac{\partial}{\partial x} \left(\alpha \frac{\partial T}{\partial x} \right) + \dot{\omega}_T(\mathbf{Y}, T) \quad (1)$$

$$\dot{m} \frac{\partial Y_k}{\partial x} = \frac{\partial}{\partial x} \left(D \frac{\partial Y_k}{\partial x} \right) + \dot{\omega}_{Y_k}(\mathbf{Y}, T) \quad (2)$$

$$(3)$$

Density is assumed to be constant (=1). The diffusivity is assumed to be constant, $\alpha = D = 1.5 \times 10^{-5}$. Auxiliary relations for the calculation of the source terms are,

$$\ddot{\omega}_{Y_k}(\mathbf{Y}, T) = \sum_{\text{reactions}} W_k \dot{\omega}_k \quad (4)$$

$$\dot{\omega}_T(\mathbf{Y}, T) = \sum_{\text{reactions}} \frac{1}{C_p} \sum_k \ddot{\omega}_{Y_k} h_k \quad (5)$$

$$\dot{\omega}_T(\mathbf{Y}, T) = \frac{Qq}{C_p} \text{(for the base case used for demo, as the above expression will lead to zero source)} \quad (6)$$

$$q = k_f \prod_k [X_k]^{\nu_{lhs,k}} - k_b \prod_k [X_k]^{\nu_{rhs,k}} \quad (7)$$

$$X_k = \frac{Y_k/W_k}{\sum_j Y_j/W_j} \quad (8)$$

$$\dot{\omega}_k = (\nu_{rhs,k} - \nu_{lhs,k}) q \quad (9)$$

The initial conditions should be carefully chosen as the solution depends on them.

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- [1] Braman, Kelvin. Parametric uncertainty and sensitivity methods for reacting flows
 - [2] Detailed and global kinetics model for hydrogen <http://www.osti.gov/scitech/servlets/purl/90098/>
 - [3] Soot Formation in Laminar Premixed Ethylene/Air Flames at Atmospheric Pressure